Assessment Plan for the Linear Alkylbenzene (LAB) Sulfonic Acids Category in Accordance with the USEPA High Production Volume Chemical Challenge Program

Prepared for:

The LAB Sulfonic Acids Coalition

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EXECUTIVE SUMMARY

The Linear Alkylbenzene (LAB) Sulfonic Acids Coalition (Coalition) is sponsoring three linear alkylbenzene sulfonic acid materials. These acids are intermediates in the manufacture of linear alkylbenzene sulfonate (LAS) surfactants, a major cleaning agent in laundry detergents. The Coalition assembled and reviewed the available public and private toxicological data, and developed an assessment plan for the sponsored materials. Because of the close structural similarity between LAS and the LAB sulfonic acids, data from LAS are included to provide supporting information for the category.

The LAB sulfonic acids are highly water soluble (miscible) and have a relatively low K_{ow}. The environmental fate data indicate that these chemicals are highly susceptible to photo- and biodegradation. The acute aquatic toxicity is consistent across the four chemicals for fish, *Daphnia*, and algae. The acute oral mammalian toxicity is similar and of low concern for all of the chemicals with available data. LAS data on the chronic aquatic toxicity, repeated dose, reproductive and developmental endpoints do not indicate any significant areas of concern for the LAB sulfonic acids.

Furthermore, the LAB sulfonic acids are exclusively used as intermediates in the production of LAS. Worker exposure potential is extremely small and highly controlled through the use of engineering controls, personal protective equipment, and use of closed production systems. There is no consumer exposure to LAB sulfonic acids since they are not used in consumer products.

Based on the availability of data and the limited exposure potential, the LAB sulfonic acids are considered to be of low concern and no further testing is necessary for the materials in the category.

INTRODUCTION

The High Production Volume (HPV) Challenge Program is a voluntary initiative of the US chemical industry to complete hazard data profiles for approximately 2800 HPV chemicals as identified on the US Environmental Protection Agency's (USEPA) 1990 Toxic Substances Control Act (TSCA) Inventory Update Rule (IUR). In the US, HPV chemicals are those that are manufactured or imported in quantities greater than 1 million pounds per year. The hazard data to be provided in the program are those that meet the requirements of the Screening Information Data Set (SIDS) Program (OECD 1997). SIDS, which has been internationally agreed to by member countries of the Organization for Economic Cooperation and Development (OECD), provides the basic screening data needed for an initial assessment of the physical-chemical properties, environmental fate, and adverse human and environmental effects of chemicals. The information for completing the SIDS can come from existing data or may be generated as part of the HPV Challenge Program. Once the available studies are identified or conducted, "robust summaries" are prepared.

The USEPA, industry, and non-governmental organizations (NGOs) are unified in their commitment to minimize the numbers of animals tested in the HPV Challenge Program whenever it is scientifically justifiable (USEPA 1999a, 2000a). One approach is to evaluate closely related chemicals as a group, or category, rather than solely as individual chemicals. The use of categories is encouraged by USEPA in the HPV Challenge Program. Appropriately constructed categories allow for a more efficient evaluation while reducing the number of animals required for testing.

The Linear Alkylbenzene (LAB) Sulfonic Acids Coalition (Coalition) has agreed to assemble and review available public and private toxicological data, develop and provide an assessment plan for the sponsored chemicals and conduct additional research, including testing when necessary, for three linear alkylbenzene sulfonic acids. These acids are intermediates in the manufacture of linear alkylbenzene sulfonate surfactants, a major cleaning agent in laundry detergents. The Coalition is comprised of the following member companies:

Colgate-Palmolive Company
Akzo Nobel Surface Chemistry LLC
The Dial Corporation
Stepan Company
Unilever HPC-USA

This assessment plan is the result of the Coalition's efforts and provides a summary and analysis of the available data, and identifies any data gaps in the SIDS data profile. Section II of this assessment plan provides a rationale and justification for the development of the LAB Sulfonic Acid category. Section III reviews the methods used in the collection of published and unpublished data. Section IV reviews the evaluation of data quality. Section V reviews the preparation of the robust summaries and the construction of a data matrix. Section VI is an in-depth evaluation of data matrix patterns for each of the four data endpoint categories (*i.e.*, physical-chemical properties, environmental fate, ecotoxicity and mammalian toxicity). Section VII is a summary of the LAB Sulfonic Acid category and its properties. Section VIII presents the conclusions regarding data availability and identifies data gaps in the SIDS profiles for the sponsored chemicals.

IDENTIFICATION OF STRUCTURE BASED CATEGORY

The LAB Sulfonic Acids Coalition is sponsoring three chemicals from the 1990 and 1994 IURs:

Benzene sulfonic acid, C_{10-16} alkyl derivatives (CAS# 68584-22-5),
Benzene sulfonic acid, dodecyl (CAS# 27176-87-0), and,
Benzene sulfonic acid, tridecyl (CAS# 25496-01-9).

Structural, process and use similarities among these substances, evaluation of existing data, and professional judgement were used to define a LAB Sulfonic Acids category for the HPV Challenge Program. The LAB Sulfonic Acids category consists of linear alkylbenzene sulfonic acid homologues with alkyl carbon chain lengths ranging from C_{10} to C_{14} and averaging 11.0 to

12.9. The primary structure is a C_{10} to C_{14} linear alkyl chain with a *para*-substituted benzene sulfonic acid group attached at any of the secondary alkyl carbon positions.

The LAB sulfonic acids are intermediates in the manufacture of linear alkylbenzene sulfonate (LAS) surfactants, a major cleaning agent for laundry detergents and other cleaning products. The feedstocks for the manufacture of the LAB sulfonic acids are linear alkyl benzenes (LAB). LAB is made by reacting a mixture of C_{10} to C_{14} n-paraffins with benzene. The alkyl attachment occurs at all but the terminal carbon positions. Consequently, LAB is a mixture of C_{10} to C_{14} linear alkyl chain homologues with average alkyl chain lengths between 11.3 and 12.6 (See Table 1) attached at any of the secondary (non-terminal) positions to the benzene ring.

LAB made in Europe has alkyl chain lengths ranging from C_{10} to C_{13} and averaging 11.6 (Valtorta et al, 2000). The alkyl chain distribution of this LAB is shown in Table 1.

Table 1

TYPICAL ALKYL CHAIN COMPOSITION*

US LAB TRADE NAMES	TYPICAL ALKYL CARBON CHAIN COMPOSITION PERCENT OF TOTAL					CALCULATED AVERAGE ALKYL CHAIN LENGTH**
	C_{10}	C_{11}	C_{12}	C_{13}	C_{14}	
Alkylate 215	15	40	40	4	<1	11.3
Nalkylene 550L	14	30	29	20	7	11.8
Alkylate 225	9	32	38	20	<1	11.6
Nalkylene 575L	9	17	28	30	15	12.2
Alkylate 229	1.5	7.5	35	46	10	12.6
European LAB***	13-14	29-34	30-32	17-21	<1	11.6
LAS	1-25	7-50	20-50	5-45	<1-10	11.7****

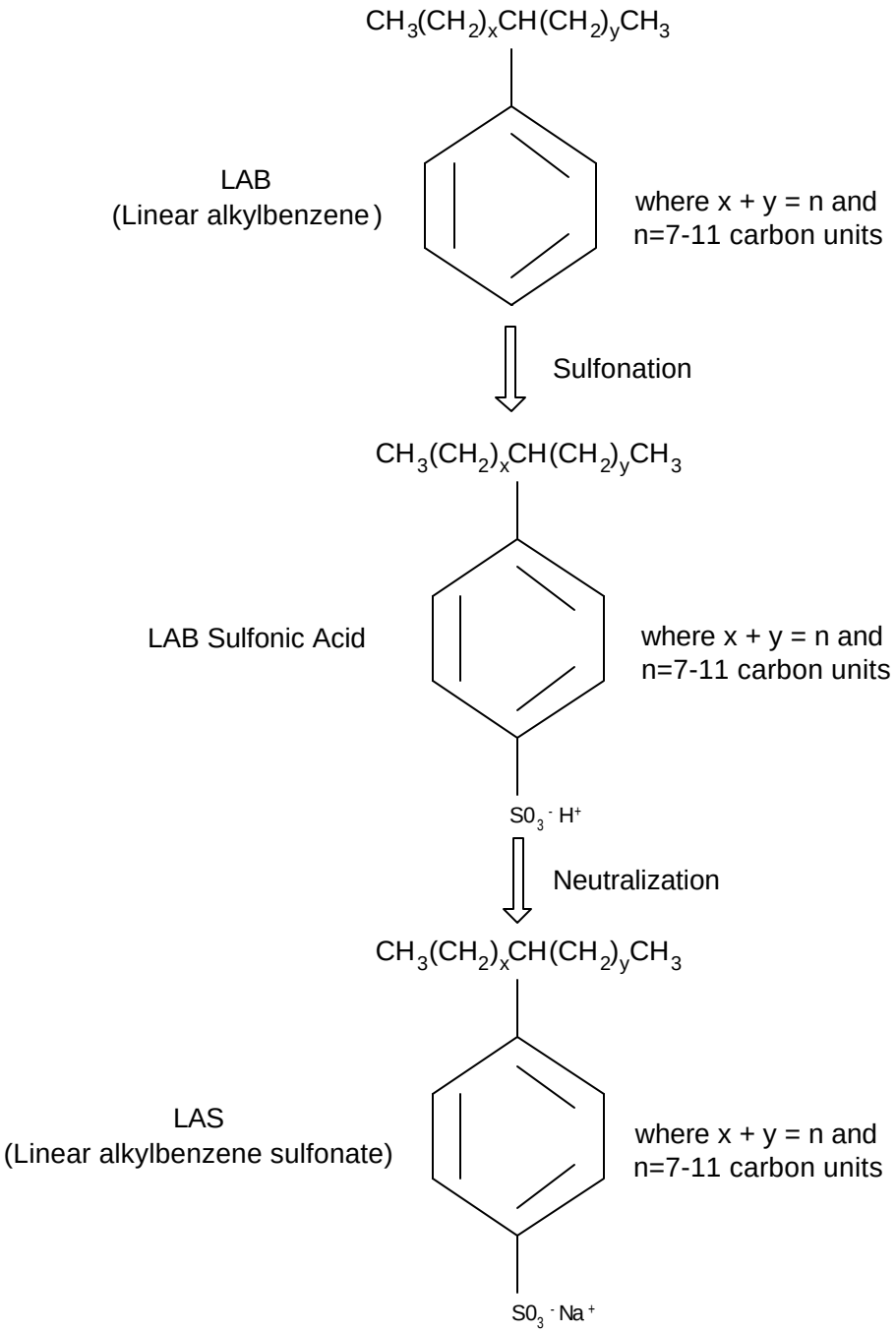
* Source: USEPA. 2002. Updated LAB SIDS report. (SIDS Initial Assessment Report (SIAR), Benzene, C10-16 Alkyl Derivatives, CAS Nos. 123-01-3, etc.)

** Calculated as $(10 \times \%C_{10}/100) + (11 \times \%C_{11}/100) + (12 \times \%C_{12}/100) + (13 \times \%C_{13}/100) + (14 \times \%C_{14}/100)$

*** Source: Valtorta et al. 2000

**** The reported average alkyl chain length for LAS is weighted by United States production volume. Data from the LAS Coalition draft Assessment Plan dated January 9, 2003.

The LAB is then reacted with SO_3 or sulfuric acid to make LAB sulfonic acids. The sulfonate group is *para* to the alkyl chain attachment on the benzene ring. The LAB sulfonic acids are, in turn, neutralized to the sodium salts, LAS. This relationship is shown below. LAB and LAS are being addressed through the SIDS program[1].



[1] An OECD SIDS assessment of LAB was completed in 1995 (the SIAP is available at www1.oecd.org/ehs/sidstable/123013.pdf). The USEPA has completed its review of a SIDS dossier and assessment report for LAS, and the LAS SIDS Consortium is currently preparing the remaining SIDS documents for submission to the USEPA in preparation for SIAM 17 (November 2003).

Although CAS# 68584-22-5 is named benzene sulfonic acid, C_{10-16} alkyl derivatives, the proportion of C_{15} and C_{16} alkyl chains in LAB is <1%, therefore, C_{10-16} LAB sulfonic acids do not contain any significant C_{15} or C_{16} constituents. In fact, alkyl chain lengths for the C_{10-16} benzene sulfonic acids range from C_{10} to C_{14} and average 11.3 to 11.8. The dodecylbenzene sulfonic acids (CAS# 27176-87-0) also are mixtures of C_{10} to C_{14} alkyl benzene sulfonic acids with average alkyl chain lengths of 11.3 to 12.6. Similarly, tridecylbenzene sulfonic acids (CAS# 25496-01-9) are mixtures of C_{10} to C_{14} alkylbenzene sulfonic acids with average alkyl chain lengths of 11.8 to 12.6. Overall, alkyl chain lengths for US-produced LAB sulfonic acids range from C_{10} to C_{14} and average from 11.3 to 12.6. The reported average alkyl chain length for LAS is 11.7, as weighted by United States production volume.

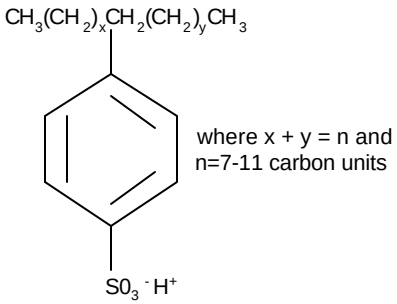
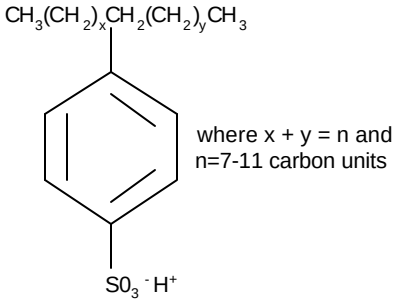
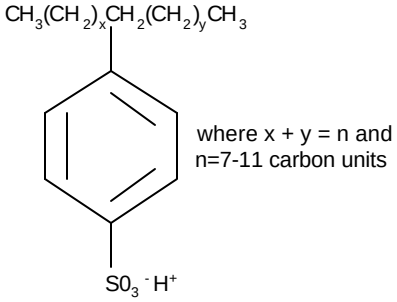
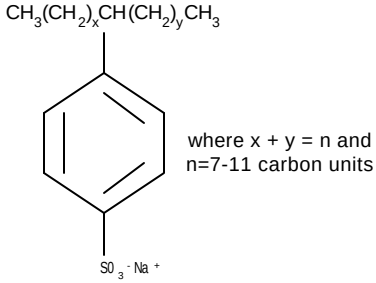
Table 2 presents the sponsored chemicals plus LAS, their CAS numbers, representative structures and average alkyl chain lengths.

Relationship of US to European LAB Sulfonic Acids

European LAB sulfonic acids (CAS # 85536-14-7) have the same alkyl chain distribution as European LAB (See Table 1), with alkyl chain lengths ranging from C_{10} to C_{13} and averaging 11.6 (Valtorta et al., 2000). European LAB sulfonic acids have an average alkyl chain distribution (11.6) in the range of those reported for the C_{10-16} LAB sulfonic acids (11.3 to 11.8). European LAB sulfonic acids have C_{14} homologue levels similar to the C_{10-16} LAB sulfonic acids (<1 to 7%). Because of the similarity of the alkyl chain distributions of European LAB sulfonic acids to those of the C_{10-16} LAB sulfonic acids, data obtained from studies of European LAB sulfonic acids (CAS # 85536-14-7) are applicable to the C_{10-16} LAB sulfonic acids (CAS # 68584-22-5).

Table 2

SPONSORED LAB SULFONIC ACIDS

COMPOUND/ MIXTURE	CAS NUMBER	REPRESENTATIVE STRUCTURE	AVERAGE ALKYL CHAIN LENGTH
Benzene sulfonic acid, C_{10-16} alkyl derivatives	68584-22-5		11.3-11.8*
Benzene sulfonic acid, dodecyl (C_{12})	27176-87-0		11.3-12.6
Benzene sulfonic acid, tridecyl (C_{13})	25496-01-9		11.8-12.6
[Supporting Substance] Linear Alkylbenzene Sulfonate (LAS)	68411-30-3 1322-98-1 25155-30-0 26248-24-8 27636-75-5 68081-81-2 85117-50-6		11.3-12.6

* Range includes European LAB sulfonic acids (CAS #85536-14-7), which have an average alkyl chain length of 11.6.

Relationship of LAB Sulfonic Acids to LAS

The LAB sulfonic acids are strong acids (pK_a <1) that are completely ionized in aqueous solutions (Lide 1990; Noller 1966). The chemical species present in aqueous solutions at neutral (physiological) pH is the LAS ion ($C_{10\text{-}14}$ linear alkyl benzene-SO_3^-), the identical species present in solutions of LAS, where the sodium ion will disassociate to form the LAS anion. Thus, the physical-chemical, environmental fate, ecotoxicity and toxicity properties of the LAB sulfonic acids and LAS would be expected to be similar. Therefore, the LAS hazard assessment data already compiled and submitted under the OECD SIDS program can be used as supporting data to supplement any LAB sulfonic acid hazard data to characterize behavior in the environment.

Use Patterns and Exposure Potential

Based on 1998 IUR data, LAB sulfonic acid production in the United States was approximately 100,000, 50,000 and 2,000 tons for CAS numbers 68584-22-5, 27176-87-0, and 25496-01-9, respectively. The carbon chain distributions of the LAB Sulfonic Acids are reflective of the carbon chain distribution of the LAB feedstock (C_{10}-C_{14}). The entire production of these LAB sulfonic acids is used as intermediates in the production of LAS. In many, but not all, cases the intermediates are site limited, *i.e.*, they remain on the production facility for use in the LAS production process. In some cases the intermediates are sold to outside LAS manufacturers. Transport to these off-site facilities is conducted following strict health and safety procedures and DOT requirements.

All processing of LAB and LAB sulfonic acids takes place in closed systems that significantly minimize worker exposure. Workers also wear standard personal protective equipment including safety goggles, face shields, safety shoes, impervious nitrile gloves, long sleeved clothing, and rubber boots. Workers may also employ cartridge-type respirators equipped with organic vapor cartridges and acid-resistant suits, for example, during steaming and washing. The closed production process and use of personal protective equipment effectively eliminates exposure to production workers. Un-ionized LAB sulfonic acid is not present after neutralization during manufacture of LAS detergent products. Therefore, no consumer exposure to LAB Sulfonic Acids from detergent use is possible.

Extensive engineering controls are in place to minimize releases to the environment. These controls include SO_2/SO_3 monitoring devices, spill containment dikes for rail unloading, leak inspections, high level tank alarms, and auto shut off valves. Emissions controls include line cyclones, electrostatic precipitation and passing through caustic scrubbers and scrubbing demisters. Some process wastewater is deep well injected. These practices and controls effectively reduce LAB sulfonic acid releases to the environment to levels far below the allowable amounts, as shown by process stack monitoring.

Based on the use patterns described above, no significant exposure to LAB sulfonic acids will occur for workers, consumers, or the environment.

COLLECTION OF UNPUBLISHED AND PUBLISHED DATA

Coalition member companies contributed in-house studies of physical-chemical properties, environmental fate and transport, ecotoxicity, and mammalian toxicity for the chemicals and mixtures in the category. To supplement the industry data, literature searches were conducted of on-line databases (*e.g.*, Hazardous Substances Databank [HSDB], Registry of Toxic Effects of Chemical Substances [RTECS], and Aquatic Toxicity Information Retrieval [AQUIRE]), standard scientific data compendia (*e.g.*, *CRC Handbook of Chemistry and Physics* and *The Merck Index*), and other published sources (*e.g.*, International Uniform Chemical Information Database [IUCLID]). The sum total of the in-house studies, reference books, and literature searches of on-line databases was the identification of a substantial amount of available data for the sponsored chemicals, which are supplemented by the data for the structurally similar LAS.

EVALUATION OF DATA FOR QUALITY AND ACCEPTABILITY

The collected data were reviewed for quality and acceptability following the general USEPA and OECD SIDS guidance (USEPA 1999b; OECD 1997) and the systematic approach described by Klimisch et al. (1997). These methods include consideration of the reliability, relevance and adequacy of the data in evaluating their usefulness for hazard assessment purposes. The Klimisch et al. (1997) approach specifies four categories of reliability for describing data adequacy. These are:

1. **Reliable without Restriction:** Includes studies or data complying with Good Laboratory Practice (GLP) procedures, or with valid and/or internationally accepted testing guidelines, or in which the test parameters are documented and comparable to these guidelines.

2. **Reliable with Restrictions:** Includes studies or data in which test parameters are documented but vary slightly from testing guidelines.

3. **Not Reliable:** Includes studies or data in which there are interferences, or that use non-relevant organisms or exposure routes, or which were carried out using unacceptable methods, or where documentation is insufficient.

4. **Not Assignable:** Includes studies or data in which insufficient detail is reported to assign a rating, *e.g.*, listed in abstracts or secondary literature.

Only those studies which are deemed reliable for the current HPV Challenge Program purposes are included in the data set for this assessment plan. Reliable studies include both categories rated 1 (Reliable without restriction) and 2 (Reliable with restrictions). Studies rated 3 (Not reliable) were not used. Studies rated 4 (Not assignable) were used when professional judgment deemed it appropriate as part of a weight-of-evidence approach. Finally, some older studies were not included if they had been superceded by more recent studies rated 1.

Much of the available data were from study reports conducted by either outside contract laboratories or in-house industry laboratories. These study reports followed standard procedures for testing of physical-chemical properties, environmental fate and transport, aquatic toxicity, and mammalian toxicity. Some of the most recent studies were conducted under GLP provisions. In addition, some data were obtained from the published, peer-reviewed, scientific literature. Reliable data from all of these sources were incorporated into the data set as appropriate. Overall, a substantial amount of data of high quality were available for chemicals and mixtures in the LAB Sulfonic Acid category.

ROBUST SUMMARIES AND CONSTRUCTION OF DATA MATRIX

Robust summaries were prepared according to the format recommended by the USEPA (1999c) and OECD (1997) and entered into the standard International Uniform Chemical Information Database (IUCLID) software. These summaries present the salient information from each of the reliable studies. All of the summaries are collected into a dossier that includes all of the individual chemicals and mixtures for the category. The robust summary dossier for the LAB Sulfonic Acid category is attached as an appendix and should be used in conjunction with this assessment plan.

Table A-1 in the Appendix to this assessment plan is a matrix of SIDS/HPV endpoints and the available data for each of the sponsored chemicals in the LAB Sulfonic Acid category. In addition, the table includes data for LAS, which support the overall predictive value of the category. Data drawn from the robust summaries are shown in the table for each endpoint and chemical when available. The data presented for LAS were derived from a dossier being developed for the OECD SIDS program and include a total of seven CAS numbers, all representative of LAS.

EVALUATION OF MATRIX DATA PATTERNS

Table A-1 identifies where data for specific compounds and data endpoints are available (data provided) and not available (indicated by "--" in the table). The available data were evaluated for patterns and trends related to structure that then could be used to predict values for a particular endpoint (*e.g.*, acute oral toxicity) where adequate data are not available (*i.e.*, "Read Across"). In addition, the data were evaluated to determine to what extent the SIDS data endpoints were covered by available data for each chemical (*e.g.*, dodecylbenzene sulfonic acid) in the category (*i.e.*, "Read Down").

Evaluation of "Read Across" Patterns

The following discussion reviews the "read across" patterns identified for each of the four major data areas: physical-chemical properties, environmental fate and transport, ecotoxicity, and mammalian toxicity.

Physical-Chemical Properties

The primary patterns in the physical-chemical properties of chemicals in the LAB Sulfonic Acids category are trends in the parameters that affect partitioning between air and water, and between water and organic phases (*e.g.*, soil or biota). The most important of these parameters are vapor pressure, water solubility, and the octanol/water partition coefficient (K_{ow}). Because of the narrow range of carbon chain lengths covered by the category, it would be expected that their physical-chemical properties would be similar.

It should be noted that the LAB sulfonic acids are liquids and LAS is a solid at room temperature. Thus, certain physical-chemical parameters are not appropriate to compare (*e.g.*, melting and boiling points). However, in water the difference between the LAB sulfonic acids and LAS disappears as dissociation results in the same ion in solution. Therefore, parameters such as K_{ow}, water solubility and pH/pK_a are appropriate to compare.

Melting and boiling point data are available for two of the LAB sulfonic acids. The IUCLID data sheet for benzene sulfonic acid, C_{10-16}-alkyl derivatives (CAS #68584-22-5) cites a Shell Chemicals report indicating a melting point of –10 ºC, consistent with materials that are liquids at room temperature. A CONDEA Vista material safety data sheet reports the same melting point value for an alkylbenzene sulfonic acid mixture. The IUCLID data sheet for dodecylbenzene sulfonic acid (CAS #27176-87-0) cites a Hoechst Iberica s.a. report with a melting point also of –10 ºC, while a standard reference compilation (Verschueren 1996) reports a melting point of 10 ºC [2]. Boiling point data for the CONDEA Vista alkylbenzene sulfonic acid mixture indicate a value of 156 ºC. The IUCLID data sheet for dodecylbenzene sulfonic acid (CAS #27176-87-0) cites a Hoechst Iberica s.a. report with a boiling point 205 ºC, while Verschueren reports a value of 315 ºC for this chemical.

The only vapour pressure information is a value of 0.22 hPa for the CONDEA Vista alkylbenzene sulfonic acid mixture. However, LAB sulfonic acids are not expected to volatilize significantly, as noted in the fugacity discussion below.

The octanol-water partition coefficients are around 2 (log K_{ow}) for all of the chemicals in this category. A Shell Chemical report cited in the IUCLID for benzene sulfonic acid, C_{10-16}-alkyl derivatives (CAS #68584-22-5) indicates a measured K_{ow} value of 2 using the

[2] Given the other available results, it is likely that this is a typographical error in the text and the actual value is –10 ºC.

Shake-Flask method. The other values are estimated using the Leo and Hansch formula and show good agreement with the measured value. Similarly, the available data indicate that all of the chemicals are very highly soluble in water, with reported values of up to 400,000 mg/L (40%).

No further testing is necessary because of the similarities between the sulfonic acids and LAS in solution.

Environmental Fate and Transport

The important information from the environmental fate data is the primary mechanism or mechanisms of degradation and whether there is any pattern to differences observed between chemicals. For organic chemicals, this is commonly the breakdown of compounds into smaller constituents by biological degradation. Other breakdown mechanisms that may be important are photolysis and hydrolysis. These breakdown mechanisms are necessarily dependent on what environmental compartment (air, water, soil, sediment) to which the chemicals are distributed. Fugacity modeling can be used to estimate the relative percentage of chemicals that will partition to various compartments at steady state. The results of the modeling using the EPI Suite of estimation programs (USEPA 2000b) are shown in Table 3.

Table 3

ENVIRONMENTAL DISTRIBUTION OF SPONSORED LAB SULFONIC ACIDS BASED ON EQC MODELING

Environmental Compartment	Benzene sulfonic acid, C10-16 alkyl derivatives*	Benzene sulfonic acid, dodecyl-	Benzene sulfonic acid, tridecyl-	[Supporting Substance] Linear Alkylbenzene Sulfonate (LAS)*
Air	1%	<1%	<1%	1%
Water	32%	29%	23%	34%
Soil	63%	60%	53%	65%
Sediment	4%	10	23%	<1%

* A C_{11} benzene sulfonic acid alkyl derivative and a C_{12} LAS were modeled for the benzene sulfonic acid, C_{10-16} alkyl derivatives and LAS, respectively because these chain lengths more closely match the average alkyl chain lengths of these materials. The model assumes a C_{12} and C_{13} alkyl chain length for the dodecyl- and tridecyl-benzene sulfonic acids, respectively. See the corresponding robust summaries for further details.

Based on physical-chemical properties, the fugacity modeling predicts that most of the sponsored chemicals will partition to the soil and water. Very little partitions to the air or sediment.

The atmospheric oxidation potential of the three sponsored chemicals in the category was estimated using the EPI Suite software (v. 3.10; USEPA 2000b). These estimations suggest that photodegradation may be a significant mechanism for the breakdown of

benzene sulfonic acids. Based on the model estimates, the hydroxyl radical reaction half-lives ranged from about 7 to 8.6 hours. Estimated data for LAS were similar. Furthermore, measured data for LAS suggest even more rapid photodegradation, with 95% of the material degraded within 20 minutes at 20 ºC in a laboratory study. With respect to stability in water, no hydrolysis information is available for the three sulfonic acids, but data do indicate that LAS is stable in water.

Measured biodegradation data are available for two of the sponsored chemicals in the category and LAS. These data indicate substantial microbial degradation under aerobic conditions. For dodecylbenzene sulfonic acid, the one available study indicates 69% of the material mineralized after 28 days[3]. Biodegradation of the C_{10-16} derivatives and the LAS are also rapid, with 93% or greater of the material degrading within 28 or 37 days. In addition, studies show that straight chain alkylbenzene sulfonate materials readily degrade, with the shorter chain length compounds degrading more rapidly (Eden et al. 1968).

Thus, the data indicate that these chemicals are highly susceptible to degradation, both by photolytic and microbial mechanisms. Available data also indicate that they have low to moderate bioaccumulation potential, with a bioconcentration factor for dodecyl benzene sulfonic acid of 130. LAS has bioconcentration factors that range from 22 to 87. No additional environmental fate studies are necessary to characterize these materials.

Ecotoxicity

The primary pattern from ecotoxicity is whether the toxicity to aquatic organisms changes predictably with structural differences in the materials. In addition, it is important to evaluate whether the physical-chemical properties of the chemicals affect their bioavailability, and subsequently, their aquatic toxicity.

Acute fish toxicity data are available for all three of the sponsored chemicals in the category and LAS. The data indicate very similar toxicity levels of these chemicals to fish, with LC_{50} values range from about 3 to 6 mg/L. Data are also available for toxicity to the invertebrate *Daphnia magna* for all four chemicals. These data similarly show a very narrow range in toxicity values, with EC_{50} values falling into a range between about 3 to 12 mg/L. Finally, data on the toxicity of three of the four chemicals to algae are also available. These data show EC_{50} values in a range from 29 to 170 mg/L. Given the complete coverage of the aquatic acute toxicity across species and the narrow ranges in results, no additional acute ecotoxicity testing is necessary. Chronic aquatic toxicity data are not required for the HPV Challenge Program. However, chronic data are available for LAS, and given that the sulfonic acids in aqueous solutions produce the identical ion as LAS, no further chronic toxicity testing is necessary.

[3] Mineralization refers to the complete degradation of the chemical to CO_2 and water. Biodegradation refers to degradation of the parent chemical into other materials, but does not necessarily include complete mineralization to CO_2 and water.

Toxicity

Toxicity to mammals is an important surrogate for estimating potential affects on humans. Again, patterns are evaluated to determine if data endpoints without values can be estimated from the data that are available. Several aspects of mammalian toxicity are evaluated. Acute testing provides information on gross effects, such as mortality, from exposure to high doses. Repeated dose testing provides information on toxicity associated with multiple doses over time. Genetic testing is conducted to evaluate the potential for mutagenic effects by using bacterial systems (*e.g.*, the Ames test), non-bacterial systems (*e.g.*, cell transformation), and in vivo (*i.e.*, live animal) systems. Reproductive and developmental/teratogenic testing provides information on the potential effects of long-term exposure to lower doses, especially as related to possible effects in developing embryos and young animals. It is important to note that the lack of significant exposure may obviate the need to fill apparent data gaps with mammalian testing.

There are three primary routes of exposure used in the evaluation of acute toxicity: 1) oral, where the test substance is introduced in food or directly into the test animal by gavage; 2) inhalation, where the substance is introduced into the lungs; and 3) dermal, where the substance is applied directly to the skin. The choice of exposure route depends on the physical-chemical characteristics of the test substance and the likely route by which animals or humans would be exposed. Data for all three routes of exposure are usually not necessary to understand the acute toxicity of a particular chemical substance.

For the LAB Sulfonic Acids category, acute oral toxicity data are available for two of the three sponsored sulfonic acids and LAS. The data indicate minimal to moderate toxicity, with LD_{50} values ranging from 500 to 2000 mg/kg body weight (bw). Acute inhalation data are available for LAS only, and indicate a lack of significant toxicity. Dermal exposure data are available for one of the LAB sulfonic acids and also indicates a lack of significant toxicity. In vitro bacterial and in vivo genetic toxicity studies are available for the C_{10-16} alkyl derivatives (CAS #68584-22-5) and these endpoints plus an in vitro non-bacterial genetic toxicity study are available for LAS. All of these studies proved negative for mutagenicity. Data on repeated dose exposures, reproductive toxicity, and developmental toxicity/teratogenicity are available for LAS and indicate a lack of significant effects on these endpoints. The data indicate that LAS is of low concern.

Besides the SIDS endpoints, data are provided on several "Beyond-SIDS" endpoints for completeness. These are endpoints that are not required by the HPV Chemical Challenge Program but are available and offer additional insight to the health and safety of the materials. For example, skin and eye irritation and sensitization potential studies are available for two of the sponsored materials and LAS. Results show that these materials can be irritating if in contact with the skin or eyes, but they were not dermally sensitizing. Carcinogenicity data for LAS indicate no differences in tumor incidence in rats with oral feed exposure for two years.

Overall, the mammalian toxicity of LAB Sulfonic Acids has been well characterized, especially when the data for LAS are considered. Results indicate a lack of significant mammalian toxicity. Data for repeated dose exposures, and reproductive and developmental endpoints are lacking for the three sponsored chemicals, but are available for LAS. Given the close relationship between LAS and the LAB Sulfonic acids, these data should suffice. In addition, the sole use of LAB sulfonic acids as intermediates in the production of LAS virtually eliminates the possibility for long-term consumer exposures. Potential occupational exposures are mitigated by the use of closed production systems and personal protective equipment. Therefore, no additional toxicity testing is deemed necessary to characterize the toxicity of the LAB Sulfonic Acids category.

Evaluation of "Read Down" Patterns

Data are available for each of the individual chemicals in the category. A complete data set is available for LAS, and, with the exception of chronic aquatic toxicity and mammalian toxicity, complete data sets are available for the three LAB Sulfonic acids. For mammalian toxicity, oral toxicity data are available for two of the three sponsored chemicals and the results are similar to the results for LAS. It is important to note that all of the LAB Sulfonic Acids are intermediates in the manufacture of LAS and LAS-related materials. Therefore there is extremely limited environmental, occupational, and commercial exposure potential. Given this limited exposure, the similarity in physical-chemical, environmental fate, ecotoxicity and toxicity data, as well as the complete data set for LAS, no additional testing is warranted.

SUMMARY OF LAB SULFONIC ACIDS CATEGORY PROPERTIES

The three sponsored chemicals are linear alkylbenzene sulfonic acids representing a range of alkyl chain lengths (C_{10}-C_{14}). They are intermediates in the manufacture of LAS, and comprise the LAB Sulfonic Acids category. Because of the close structural similarity between LAS and the LAB sulfonic acids, data from LAS are included to provide supporting information for the category. All of the relevant physical-chemical properties are similar between the chemicals. They are highly water soluble (miscible) and have a relatively low K_{ow}.

The environmental fate data indicate that these chemicals are highly susceptible to photo- and biodegradation. The acute aquatic toxicity is consistent across the four chemicals for fish, *Daphnia*, and algae. Similarly, acute oral mammalian toxicity is similar and of low concern for all of the chemicals with available data. LAS data on the chronic aquatic toxicity, repeated dose, reproductive and developmental endpoints do not indicate any significant areas of concern.

Table 4 shows the availability of data and assessment plan status for the LAB Sulfonic Acids category.

CONCLUSIONS

Substantial data are available for the three sponsored LAB sulfonic acids and LAS, the supporting substance. These data show consistent results across the LAB sulfonic acids category and are generally not a toxicological concern. Furthermore, the LAB sulfonic acids are exclusively used as intermediates in the production of LAS. Worker exposure is extremely limited and highly controlled through the use of engineering controls, personal protective equipment, and use of closed production systems. There is no consumer exposure to LAB sulfonic acids since they are not used in consumer products.

Based on the availability of data and the limited exposure potential, the LAB sulfonic acids are considered to be of low concern and no further testing is necessary for the materials in the category.

Table 4

DATA AVAILABILITY AND ASSESSMENT PLAN STATUS FOR THE LAB SULFONIC ACID CATEGORY

	Data Available	Data Acceptable	Testing Required
Physical-Chemical Properties			
Melting Point	Y	Y	N
Boiling Point	Y	Y	N
Vapor Pressure	Y	Y	N
Octanol/Water Partition Coefficient	Y	Y	N
Water Solubility	Y	Y	N
pH Value, pK_a Value	Y	Y	N
Environmental Fate and Pathways			
Photodegradation	Y	Y	N
Stability in Water	Y *	Y	N
Biodegradation	Y	Y	N
Bioaccumulation	Y	Y	N
Ecotoxicity			
Acute/Prolonged Toxicity to Fish	Y	Y	N
Acute Toxicity to *Daphnia*	Y	Y	N
Toxicity to Aquatic Plants (algae)	Y	Y	N
Chronic Toxicity to Fish	Y *	Y	N
Chronic Toxicity to Aquatic Invertebrates	Y *	Y	N
Toxicity			
Acute Oral Toxicity	Y	Y	N
Acute Inhalation Toxicity	Y *	Y	N
Acute Dermal Toxicity	Y	Y	N
Skin Irritation	Y	Y	N
Eye Irritation	Y	Y	N
Skin Sensitization	Y	Y	N
Repeated Dose Toxicity	Y *	Y	N
Genetic Toxicity in vitro (Bacterial test)	Y	Y	N
Genetic Toxicity in vitro (Non-bacterial test)	Y *	Y	N
Genetic Toxicity in vivo	Y	Y	N
Carcinogenicity	Y *	Y	N
Toxicity to Reproduction	Y *	Y	N
Developmental Toxicity	Y *	Y	N

* Surrogate data available for the supporting substance Linear Alkylbenzene Sulfonate (LAS)

REFERENCES

Eden, G.E., Truesdale, G.A., and Stennett, G.V. 1968. Assessment of bioavailability. Wat. Pollut. Control. pp.107-123.

Klimisch, H.-J., Andreae, M., and Tillmann, U. 1997. A systematic approach for evaluating the quality of experimental toxicological and ecotoxicological data. Regul. Toxicol. Pharmacol. 25:1-5.

Lide, D.R. 1990. Handbook of Chemistry and Physics. 71st Edition. Ann Arbor: CRC Press.

Noller, C.R. 1966. Textbook of Organic Chemistry. Third Edition. Philadelphia: W.B. Saunders Company.

OECD. 1997. SIDS Manual (third revision). Organization for Economic Cooperation and Development. July 1997.

USEPA. 1999a. HPV Chemical Human Health Testing: Animal Welfare Issues and Approaches. Guidance document dated February 1999.

USEPA. 1999b. Determining the Adequacy of Existing Data. Draft guidance document dated February 10, 1999.

USEPA. 1999c. Draft Guidance on Developing Robust Summaries. October 22, 1999.

USEPA. 2000a. Chemical Right to Know High Production Volume Challenge Program: Fact Sheet on Animal Welfare. July 2000. EPA 745-F-99-003.

USEPA. 2000b. EPI Suite Estimation Software, v. 3.10.

Valtorta, L., Radici, P., Calcinai, D., and Cavalli, L. 2000. Recent development of LAB/LAS. La Rivista Italiana Delle Sostanze Grasse 77:73-76.

Verschueren, K. 1996. Handbook of Environmental Data on Organic Chemicals. Third Edition. New York: John Wiley & Sons, Inc.

Table A-1

Summary of Data Available for the LAB Sulfonic Acids

Section	Description	Benzene sulfonic acid, C10-16-alkyl derivatives	Benzene sulfonic acid, dodecyl-	Benzene sulfonic acid, tridecyl-	[Supporting Substance] Linear Alkylbenzene Sulfonate (LAS)
	CAS Number	**68584-22-5**	**27176-87-0**	**25496-01-9**	**68411-30-3 et al.**
	Physical-Chemical Data				
2.1	Melting Point	<-10°C	10°C	--	198.5°C
2.2	Boiling Point	156°C	315°C, 205°C	--	Decomposition onset at 444°C
2.4	Vapour Pressure	0.22 hPa	--	--	3×10^{-13} Pa
2.5	Octanol/Water Partition Coefficient (log)	2.0 at 23°C	1.96	2.52	3.32
2.6.1	Water Solubility	Miscible up to 40% (4×10^5 mg/L at 20°C)	3×10^5 mg/L at 20°C	--	2.5×10^5 mg/L at 20°C
	pH Value, pKa Value	pKa < 1	pKa < 1	pKa < 1	pH = 10 (1% solution)
	Environmental Fate and Pathways				
3.1.1	Photodegradation	$t_{1/2}$ = 8.6 hrs	$t_{1/2}$ = 7.9 hrs	$t_{1/2}$ = 7.2 hrs	>95% after 20 minutes
3.1.2	Stability in Water	--	--	--	stable
3.5	Biodegradation	94% biodegradation after 28 days* 92% biodegradation after 37 days*	69% mineralization after 28 days	--	93% after 28 days
3.7	Bioaccumulation	--	3-day BCF(fish) = 130	--	BCF = 22-87
	Ecotoxicity				
4.1	Acute/Prolonged Toxicity to Fish	96-h LC_{50}=5.6 mg/L*	96-h LC_{50}=4.1, 10, 4.3 mg/L	96-h LC_{50}=3 mg/L	96-h LC_{50} = 5.8 mg/L LC_{50} = 3.0-3.2 mg/L
4.2 A	Acute Toxicity to Daphnia	48-h EC_{50}=5.2 mg/L* 48-h EC_{50}=9.3-11.6 mg/L 48-h EC_{50}=2.9 mg/L	EC_{50}=12, 5.88 mg/L	48-h EC_{50}=4.3 mg/L	48-h EC_{50} = 6.8 mg/L EC_{50} = 4.1-4.7 mg/L
4.3	Toxicity to Aquatic Plants (e.g., algae)	72-h EC_{50}=36 mg/L* EC_{50}=170 mg/L	EC_{50}=50, 29 mg/L		72-h EC_{50} = 163 mg/L IC_{50} = 9.1 mg/L
4.5.1	Chronic Toxicity to Fish	--	--	--	NOEC = 0.25-3.2 mg/L
4.5.2	Chronic Toxicity to Aquatic Invertebrates	--	--	--	NOEC = 1.4 mg/L
	Toxicity				
5.1.1	Acute Oral Toxicity	LD_{50} (rat) = 1,470 mg/kg bw* LD_{50} (rat) = 775 mg/kg bw	LD_{50} (rat) = 500-2,000 mg/kg bw	--	LD_{50} (rat) = 1,080-1,980 mg/kg bw
5.1.2	Acute Inhalation Toxicity	--	--	--	LC_{50} = 310 mg/m^3 particulate
5.1.3	Acute Dermal Toxicity	LD_{50} (rabbit) = 2,000 mg/kg bw	--	--	LD_{50} (rat, rabbit) >2000 mg/kg bw
5.2.1	Skin Irritation	irritating at 0.5 mL*	irritiating at 0.5 mL	--	irritating
5.2.2	Eye Irritation	irritating at 0.1 mL*	--	--	irritating
5.3	Sensitization	no sensitizing potential	--	--	not sensitizing
5.4	Repeated Dose Toxicity	--	--	--	NOAEL (rat) = 85 mg/kg bw
5.5	Genetic Toxicity *in vitro* (Bacterial test)	non-genotoxic	--	--	non-genotoxic
5.5	Genetic Toxicity *in vitro* (Non-bacterial test)	--	--	--	non-genotoxic
5.6	Genetic Toxicity *in vivo*	non-genotoxic*	--	--	non-genotoxic
5.7	Carcinogenicity	--	--	--	NOAEL (rat) = 250 mg/kg bw d
5.8	Toxicity to Reproduction	--	--	--	NOAEL (rat) = 350 mg/kg bw d
5.9	Developmental Toxicity/Teratogenicity	--	--	--	NOAEL (rat, oral) = 780 mg/kg bw d NOAEL (mouse, dermal) = 1500 mg/kg bw d

-- No data available
bw = body weight
* Data from European LAB sulfonic acid (CAS #85536-14-7) used as a surrogate.